Layered catalytic reactors for direct natural gas conversion to ethylene

Laura Pirro, Joris De Keulenaer*, Pedro S.F. Mendes*, Bart D. Vandegehuchte**, Guy B. Marin*, Joris W. Thybaut**

**Laboratory for Chemical Technology, Ghent University*
***Total Research and Technology Feluy*

Direct natural gas conversion into C_2 products, i.e., ethane and ethylene, via the Oxidative Coupling of Methane (OCM) reaction, represents one of the most interesting, but at the same time complex, challenges in the field of heterogeneous catalysis [1]. In the attempt to develop an industrially profitable solution for this process, layered fixed-bed reactors are regarded as a promising alternative [2]. Such a configuration would allow, for instance, a first layer of active catalyst, that can more easily activate methane, followed by a layer of selective catalyst, that minimizes the oxidation of the desired C_2 products [3], hence, increasing the overall yield. Despite the attractiveness of this layered reactor concept for OCM, limited research has been performed on the topic and the so far unsatisfactory understanding of this configuration has prevented further optimization and scale up.

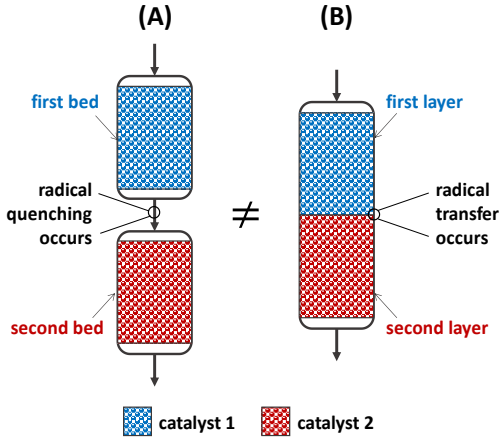

Figure 1. Schematic representation of catalytic reactors in series (A) and catalytic layers in series.

Microkinetic simulations are considered as a promising tool in the analysis and optimization of OCM layered fixed-bed reactors, thanks to the possibility of *in silico* assessing the impact of operating conditions, catalyst properties and bed composition on the ultimate C_2 yield. For this purpose, a comprehensive microkinetic model previously developed in this research group [4], including both gas phase and surface reactions, was herein adopted.

As depicted in Figure 1, two configurations of a layered fixed bed setup are possible: a series of fixed-bed reactors (A) or a sequence of two catalyst layers within the same fixed-bed reactor (B). In the case of OCM, for the former (A), radical quenching occurs between two consecutive reactors, and the active gas phase species generated in the first bed are thus considered to be inactive at the inlet of the second catalyst bed. In the case of a single reactor (B), the contribution of radical transfer is taken into account and might result in enhanced activity in the second catalytic layer.

In order to adequately simulate consecutive layers of catalysts (B), an in-house fixed-bed reactor model [6] was customized, by explicitly including radical species in the boundary conditions of the set of Partial Differential Equations which are solved in each layer. An extensive simulation campaign is currently ongoing with the customized model, aiming at improving C_2 yields via optimization of operating conditions and bed composition.
The deeper understanding being gained in this work is believed to be a necessary step in the quest for a profitable industrial OCM process.

References:
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E-mail: laura.pirro@ugent.be; Website: https://www.lct.ugent.be/research